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Application of class $\mathscr{S}_m$ variable transformations to numerical integration over surfaces of spheres

Avram Sidi*

Computer Science Department, Technion - Israel Institute of Technology, Haifa 32000, Israel

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Abstract

Class $\mathscr{S}_m$ variable transformations with integer m for finite-range integrals were introduced by the author (Numerical Integration IV, International series of Numerical Mathematics, Basel, 1993, pp. 359–373) about a decade ago. These transformations "periodize" the integrand functions in a way that enables the trapezoidal rule to achieve very high accuracy, especially with even m. In a recent work by the author (Math. Comp. (2005)), these transformations were extended to *arbitrary* m, and their role in improving the convergence of the trapezoidal rule for different classes of integrands was studied in detail. It was shown that, with m chosen appropriately, exceptionally high accuracy can be achieved by the trapezoidal rule. In the present work, we make use of these transformations in the computation of integrals on surfaces of spheres in conjunction with the product trapezoidal rule. We treat integrands that have point singularities of the single-layer and double-layer types. We propose different approaches and provide full analyses of the errors incurred in each. We show that surprisingly high accuracies can be achieved with suitable values of m. We also illustrate the theoretical results with numerical examples. Finally, we also recall analogous procedures developed in another work by the author (Appl. Math. Comput. (2005)) for regular integrands.

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* Tel.:/fax: +972 4 8294364.
E-mail address: asidi@cs.technion.ac.il.

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1. Introduction

The numerical computation of integrals, of functions with point singularities, on surfaces of bounded domains in $\mathbb{R}^3$ is a task frequently encountered in applications. Such integrals arise naturally in boundary integral formulations of continuum problems in $\mathbb{R}^3$, and the relevant singularities are of the single- and double-layer types. For a review of this subject, see, for example, Atkinson [1], [2, Chapter 5].

In the present work, we consider the computation of such integrals on surfaces of spheres. Without loss of generality, we consider integrals over the surface of the unit sphere, denoted U,

$$U := \{(x, y, z) : \quad x^2 + y^2 + z^2 = 1\}. \tag{1.1}$$

The integrals we wish to treat then are of the form

$$I[f] = \int\int_U f(Q)\,\mathrm{d}A, \qquad Q = (x, y, z) \in U, \tag{1.2}$$

where dA is the associated area element on U. The integrands $f(Q)$ are either of the form

$$f(Q) = \frac{g(Q)}{|Q - P|}, \qquad P \in U \text{ (single-layer)}, \tag{1.3}$$

or of the form

$$f(Q) = \frac{g(Q)\,[(Q - P)\bullet\mathbf{n}_Q]}{|Q - P|^3}, \qquad P \in U \text{ (double-layer)}, \tag{1.4}$$

where $g(Q)$ is smooth over U, $|Q - P|$ denotes the Euclidean distance between P and Q, $\mathbf{n}_Q$ is the outward normal to U at Q, and $(Q - P)\bullet\mathbf{n}_Q$ is the dot product of the vectors $(Q - P)$ and $\mathbf{n}_Q$. We let $P = (x_0, y_0, z_0)$ in the sequel.

Here are the steps of the basic numerical approach for computing $I[f]$ that we propose in this work:

(i) Rotate the coordinate system on U such that either the north pole or the south pole is mapped to P, the point of singularity of $f(Q)$ on U. (How this can be done will be described shortly.)

(ii) Express the (transformed) integral over U in terms of the standard spherical coordinates θ and ϕ, $0 \leqslant \theta \leqslant \pi$ and $0 \leqslant \phi \leqslant 2\pi$. The resulting integral can be written in the form $I[f] = \int_0^{\pi}[\int_0^{2\pi} F(\theta, \phi)\,\mathrm{d}\phi]\,\mathrm{d}\theta$.

(iii) Transform θ by an appropriate periodizing variable transformation $\theta = \Psi(t)$, $0 \leqslant t \leqslant 1$. Here, $\Psi(t)$ is derived from a standard variable transformation $\psi(t)$ in the extended class $\mathscr{S}_m$ of Sidi [10], with m chosen suitably. (We will discuss how this is done shortly.) The result of this is $I[f] = \int_0^1[\int_0^{2\pi} F(\Psi(t), \phi)\,\mathrm{d}\phi]\Psi'(t)\,\mathrm{d}t$.

(iv) Approximate the final integral in the variables t and ϕ by the product trapezoidal rule.

Note: The basic method above, although quite effective as is, can be improved substantially by applying it to $I[f - r]$ for some suitably (and simply) chosen function $r(Q)$, such that $I[r]$ is much less expensive to compute than $I[f]$. We will discuss the details of this improved procedure later.

The essentials of the approach we have just presented can be found in the recent paper [11], which treats integrals of nonsingular functions over smooth surfaces that are homeomorphic to the surface of the unit sphere. This paper presents a discussion on the merits of employing variable transformations in general. In addition, it provides the definition and a summary of the properties of transformations in the extended classes $\mathscr{S}_m$, and also the $\sin^m$-transformation in $\mathscr{S}_m$ that we have used in our computations. Finally, it also provides the relevant Euler–Maclaurin expansions, including an extension of them due to Sidi [9]. All these comprise the analytical tools necessary for the study of the methods of the present work. In the sequel, we will refer freely to [11,10] for these tools.

We now turn to the complete mathematical description of the basic approach we have sketched above; we also explain how the coordinate system can be rotated in a simple way and how $\Psi(t)$ is constructed.

The transformation of the (x, y, z) coordinate system such that the point $P = (x_0, y_0, z_0)$ is mapped to the north pole or the south pole of U can be carried out by mapping U onto itself (orthogonally) via a fixed 3×3 real orthogonal matrix H (that is, $H^{-1} = H^{\mathrm{T}}$) such that

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = H \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix}, \quad \begin{bmatrix} x_0 \\ y_0 \\ z_0 \end{bmatrix} = \mu H e_3; \quad \mu = \pm 1, \quad e_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \tag{1.5}$$

Here μ should be chosen in a way that does not cause loss of accuracy numerically. For example, following Atkinson [3], we can take H to be a real Householder matrix, with μ fixed such that H is computed in the most stable way possible: When $z_0 \neq 0$,

$$\mu = -\mathrm{sgn}(z_0); \quad H = I - 2pp^{\mathrm{T}}, \quad p = \frac{1}{\sqrt{2 + 2|z_0|}} \begin{bmatrix} x_0 \\ y_0 \\ \mathrm{sign}(z_0)(|z_0| + 1) \end{bmatrix} \tag{1.6}$$

and when $z_0 = 0$, we have

$$\mu = +1 \ \text{ or } \ \mu = -1; \quad H = I - 2pp^{\mathrm{T}}, \quad p = \frac{1}{\sqrt{2}} \begin{bmatrix} x_0 \\ y_0 \\ -\mu \end{bmatrix}. \tag{1.7}$$

(Recall that, if H is a real Householder matrix, then it is symmetric, and hence satisfies $H^{-1} = H$, in addition to $H^{-1} = H^{\mathrm{T}}$.)

We now propose a procedure that enables us to use only (1.6) for determining $H = I - 2pp^{\mathrm{T}}$, $p^{\mathrm{T}}p = 1$. Letting $\rho = \max\{|x_0|,\ |y_0|,\ |z_0|\}$, so that $\rho \geqslant 1/\sqrt{3} > 0$, we consider three separate cases:

(i) If $|x_0| = \rho$, then

$$\begin{bmatrix} y \\ z \\ x \end{bmatrix} = H \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix}, \quad \begin{bmatrix} y_0 \\ z_0 \\ x_0 \end{bmatrix} = -\mathrm{sign}(x_0) H e_3; \quad p = \frac{1}{\sqrt{2+2|x_0|}} \begin{bmatrix} y_0 \\ z_0 \\ \mathrm{sign}(x_0)(|x_0|+1) \end{bmatrix}. \tag{1.8}$$

(ii) If $|y_0| = \rho$, then

$$\begin{bmatrix} z \\ x \\ y \end{bmatrix} = H \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix}, \quad \begin{bmatrix} z_0 \\ x_0 \\ y_0 \end{bmatrix} = -\mathrm{sign}(y_0) H e_3; \quad p = \frac{1}{\sqrt{2+2|y_0|}} \begin{bmatrix} z_0 \\ x_0 \\ \mathrm{sign}(y_0)(|y_0|+1) \end{bmatrix}. \tag{1.9}$$

(iii) If $|z_0| = \rho$, then

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = H \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix}, \quad \begin{bmatrix} x_0 \\ y_0 \\ z_0 \end{bmatrix} = -\mathrm{sign}(z_0) H e_3; \quad p = \frac{1}{\sqrt{2+2|z_0|}} \begin{bmatrix} x_0 \\ y_0 \\ \mathrm{sign}(z_0)(|z_0|+1) \end{bmatrix}. \tag{1.10}$$

Note that, in these transformations, x, y, z are permuted cyclically to preserve the orientation of the coordinate system.

Following this mapping of U onto itself, introduce the standard spherical coordinates θ and ϕ, via

$$(\tilde{x}, \tilde{y}, \tilde{z}) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta); \quad 0 \leqslant \theta \leqslant \pi, \quad 0 \leqslant \phi \leqslant 2\pi. \tag{1.11}$$

Then,

$$I[f] = \int_0^{\pi} \left[\int_0^{2\pi} F(\theta, \phi)\, d\phi \right] d\theta, \quad F(\theta, \phi) = f(x, y, z)\sin\theta, \tag{1.12}$$

(x, y, z) being related to (θ, ϕ) through (1.5) and (1.11). As is known, and as we will see shortly, $F(\theta, \phi)$ is infinitely differentiable for all $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$.

As for the variable transformation $\Psi(t)$, we wish to propose two essentially different ways for doing this. Of these, the first is the standard way of using variable transformations. The second, introduced first in [7,10], and used in [11], is quite unusual; however, it turns out to be more effective numerically than the first, in addition to being interesting theoretically.

1. Choose $\Psi(t) = \Psi_1(t) = \pi\psi(t)$, where $\psi(t)$ is a transformation in the class $\mathscr{S}_m$.
2. When P is mapped to the south pole, that is, $\mu = -1$ in (1.5), choose $\Psi(t) = \Psi_2(t) = 2\pi\psi(t/2)$. When P is mapped to the north pole, that is, $\mu = +1$, in (1.5), choose $\Psi(t) = \Psi_2(t) = \pi[2\psi((1+t)/2) - 1]$. Again, $\psi(t)$ is a transformation in the class $\mathscr{S}_m$.

Then, the transformed integral becomes

$$I[f] = \int_0^{1} \left[\int_0^{2\pi} \widehat{F}(t, \phi)\, d\phi \right] dt; \quad \widehat{F}(t, \phi) = F(\Psi(t), \phi)\Psi'(t). \tag{1.13}$$

Finally, this integral is approximated via the product trapezoidal rule

$$\widehat{T}_{n,n'}[f] = hh' {\sum_{j=0}^{n}}'' \sum_{k=1}^{n'} \widehat{F}(jh, kh'); \quad h = \frac{1}{n}, \quad h' = \frac{2\pi}{n'}, \tag{1.14}$$

where n and n' are positive integers, and the double prime on a summation means that the first and the last terms in the summation are to be multiplied by 1/2. We let $n' \sim \alpha n^{\beta}$ as $n \to \infty$ for some fixed positive α and β in the sequel.

Note that the product trapezoidal rule for an arbitrary integral $\int_0^1 [\int_0^{2\pi} \widehat{F}(t, \phi)\, d\phi] dt$, where $\widehat{F}$ is continuous for $(t, \phi) \in [0, 1] \times [0, 2\pi]$, is actually $hh' \sum''^{n}_{j=0} \sum''^{n'}_{k=0} \widehat{F}(jh, kh')$. $\widehat{T}_{n,n'}[f]$ in (1.14) becomes the product trapezoidal rule in our case because $F(\theta, \phi)$, and hence also $\widehat{F}(t, \phi)$, are 2π-periodic in ϕ.

The variable transformations $\theta = \Psi(t)$ above turn out to be very effective in that the accuracy of $\widehat{T}_{n,n'}[f]$ increases with increasing m, and in a subtle way. For some special values of m, unusually high accuracies are achieved, as we will see later. Also, as mentioned already, the transformation $\Psi_2(t)$ produces more accuracy than $\Psi_1(t)$ for the same value of m. In addition, its performance can be improved further by subtracting from $f(Q)$ a simple known function.

The plan of this paper is as follows:

At the end of this section, we reproduce the definition of the extended class $\mathscr{S}_m$, and describe briefly the $\sin^m$-transformation that is in this class and that we have used in our computations. In the next section, we present some preliminary results concerning the structure of $f(Q)$ and of the rule $\widehat{T}_{n,n'}[f]$ in the presence of the point singularities in (1.3) and (1.4). In Section 3, we analyze the asymptotic behavior of $F(\theta, \phi)$ and of the integral $v(\theta) = \int_0^{2\pi} F(\theta, \phi)\, d\phi$ as $\theta \to 0$ and $\theta \to \pi$. The main results of this section are Theorems 3.1 and 3.2, and they concern $v(\theta)$.

In Section 4, we give the analysis of the basic rules described in the present section and provide numerical examples in which these rules are used. Theorems 4.1 and 4.2 are the main results of this section. Theorem 4.1 shows that, with the variable transformation $\theta = \Psi_1(t)$, the error in the basic rule is at worst $O(h^{2m+2})$ provided m is an even integer, while Theorem 4.2 shows that, with $\theta = \Psi_2(t)$, the error is at worst $O(h^{4m+4})$ provided $2m$ is an odd integer.

In Section 5, we give an improvement of the basic rule that uses the variable transformation $\theta = \Psi_2(t)$; we apply the rule $\widehat{T}_{n,n'}$ after preprocessing $f(Q)$. We approximate $I[f]$ by $\widehat{T}_{n,n'}[f - r] + I[r]$, where $f(Q) - r(Q)$ is determined by subtracting from $g(Q)$ the constant $g(-P)$, and $I[r]$ is known analytically. The error in this case turns out to be at worst $O(h^{6m+6})$ provided $4m$ is an odd integer, as shown in Theorem 5.1. We provide a numerical example in this case too.

For the sake of completeness, in Section 6, we recall the numerical integration methods of [11] for regular integrands over the surface of the unit sphere and summarize their relevant theory.

For the high-accuracy cases in Theorems 4.1, 4.2, and 5.1, and for the high-accuracy case in Section 6, we also provide the complete asymptotic expansions of the errors.

We would like to mention that the results of Theorems 3.1 and 3.2 form the basis for the lines of thought leading to the design of the numerical integration rules described in Theorems 4.2 and 5.1.

At this point, we would like to note that, in case the integration is defined over an arbitrary smooth surface S in $\mathbb{R}^3$ that is homeomorphic to U, we first map S to U, and continue as above. The details of the method and its rigorous analysis are much more complicated in this case, however.

Before closing, we mention that our basic method that uses the transformation $\theta = \Psi_1(t)$ and that is treated in Theorem 4.1 is analogous to a recent method of Atkinson [3], and its numerical performance is very similar to that of [3] as well. There are no analogues of our improved methods and their corresponding theory, namely, of our Theorems 4.2 and 5.1, in [3], however. One of the major differences between the methods of the present paper and that of [3] is that in the present paper, the variable θ on the unit sphere is transformed (by a variable transformation related to one in the extended class $\mathscr{S}_m$), whereas in [3], θ is "graded" in a special and interesting way by the introduction of a grading parameter, instead of being transformed.

Finally, this paper is partly based on the report [7] by the author.

1.1. The extended class $\mathscr{S}_m$ and the $\sin^m$*-transformation*

Definition 1.1. A function $\psi(t)$ is in the *extended class* $\mathscr{S}_m$, m arbitrary, if it has the following properties:

1. $\psi \in C[0, 1]$ and $\psi \in C^\infty(0, 1)$; $\psi(0) = 0$, $\psi(1) = 1$, and $\psi'(t) > 0$ on $(0, 1)$.
2. $\psi'(t)$ is symmetric with respect to $t = 1/2$; that is, $\psi'(1-t) = \psi'(t)$. Consequently, $\psi(1-t) = 1 - \psi(t)$.

3. $\psi'(t)$ has the following asymptotic expansions as $t \to 0+$ and $t \to 1-$:

$$\psi'(t) \sim \sum_{i=0}^{\infty} \varepsilon_i t^{m+2i} \quad \text{as } t \to 0+; \quad \psi'(t) \sim \sum_{i=0}^{\infty} \varepsilon_i (1-t)^{m+2i} \quad \text{as } t \to 1-, \tag{1.15}$$

   the ε_i being the same in both expansions, and $\varepsilon_0 > 0$. Consequently,

$$\psi(t) \sim \sum_{i=0}^{\infty} \varepsilon_i \frac{t^{m+2i+1}}{m+2i+1} \quad \text{as } t \to 0+,$$
$$\psi(t) \sim 1 - \sum_{i=0}^{\infty} \varepsilon_i \frac{(1-t)^{m+2i+1}}{m+2i+1} \quad \text{as } t \to 1-. \tag{1.16}$$

4. Furthermore, for each positive integer k, $\psi^{(k)}(t)$ has asymptotic expansions as $t \to 0+$ and $t \to 1-$ that are obtained by differentiating those of $\psi(t)$ term by term k times.

The most important property of transformations in the extended class $\mathscr{S}_m$ is that the consecutive powers of t and $(1-t)$ in their asymptotic expansions increase by 2 instead of by 1.

A representative of this class, which we use in our computations too, is the $\sin^m$-transformation that was first introduced in [6] for integer m. This transformation, just as the original $\sin^m$-transformation, is defined via

$$\psi_m(t) = \frac{\Theta_m(t)}{\Theta_m(1)}; \quad \Theta_m(t) = \int_0^t (\sin \pi u)^m \, du. \tag{1.17}$$

From the equality

$$\Theta_m(t) = \frac{m-1}{m}\Theta_{m-2}(t) - \frac{1}{\pi m}(\sin \pi t)^{m-1} \cos \pi t,$$

which can be obtained by integration by parts, we have the recursion relation

$$\psi_m(t) = \psi_{m-2}(t) - \frac{\Gamma(m/2)}{2\sqrt{\pi}\Gamma((m+1)/2)}(\sin \pi t)^{m-1} \cos \pi t. \tag{1.18}$$

Here $\Gamma(z)$ is the Gamma function. Note that $\psi_m(t)$ is related to $\psi_{m-2}(t)$ but not to $\psi_{m-1}(t)$.

When m is a positive integer, $\psi_m(t)$ can be expressed in terms of elementary functions. In this case, $\psi_m(t)$ can be computed via (1.18), with the initial conditions

$$\psi_0(t) = t \quad \text{and} \quad \psi_1(t) = \tfrac{1}{2}(1 - \cos \pi t). \tag{1.19}$$

When m is not an integer, $\psi_m(t)$ cannot be expressed in terms of elementary functions. It can be expressed conveniently in terms of hypergeometric functions, however. By the fact that $\Theta_m'(t) = (\sin \pi t)^m$ is symmetric with respect to $t = 1/2$, we have that $\Theta_m(t) = \Theta_m(1) - \Theta_m(1-t)$ for $t \in [1/2, 1]$ and thus $\Theta_m(1) = 2\Theta_m(1/2)$ as well. Thus, it is enough to know $\Theta_m(t)$ for $t \in [0, 1/2]$. Consequently,

$$\psi_m(t) = \frac{\Theta_m(t)}{2\Theta_m(1/2)} \text{ for } t \in [0, 1/2]; \quad \psi_m(t) = 1 - \psi_m(1-t) \text{ for } t \in [1/2, 1]. \tag{1.20}$$

Therefore, it is enough to consider the computation of $\Theta_m(t)$ only for $t \in [0, 1/2]$. One of the representations in terms of hypergeometric functions now reads

$$\Theta_m(t) = \frac{(2S)^{m+1}}{\pi(m+1)} F\left(\frac{1}{2} - \frac{1}{2}m, \frac{1}{2}m + \frac{1}{2}; \frac{1}{2}m + \frac{3}{2}; S^2\right); \quad S = \sin\frac{\pi t}{2}, \tag{1.21}$$

which has the convergent expansion

$$\Theta_m(t) = \frac{(2S)^{m+1}}{\pi} \sum_{k=0}^{\infty} \frac{((1-m)/2)_k}{k!} \frac{S^{2k}}{m+2k+1}; \quad S = \sin\frac{\pi t}{2}. \tag{1.22}$$

Now, the terms in this expansion are all of the same sign for $k \geqslant \lfloor (m+1)/2 \rfloor$. In addition, the kth term is $O(k^{-(m+3)/2}S^{2k})$ as $k \to \infty$ and, by the fact that $0 \leqslant S \leqslant \sin(\pi/4) = 1/\sqrt{2}$ when $t \in [0, 1/2]$, it is $O(k^{-(m+3)/2}2^{-k})$ at worst. This gives us a quickly converging expansion for $\Theta_m(t)$ that can be used conveniently for the actual computation of $\Theta_m(t)$. Furthermore, the convergence of this series can be accelerated by applying to it a suitable nonlinear sequence transformation such as that of Shanks [5] (or the equivalent ε-algorithm of Wynn [12]) or that of Levin [4]. Both transformations are treated in detail in the recent book by Sidi [8].

2. Preliminary results

In this section, we give some preliminary results concerning the structure of $F(\theta, \phi)$ and $\widehat{T}_{n,n'}[f]$.

We begin with $F(\theta, \phi)$. We consider the case $\mu = +1$ in (1.5) in detail, the treatment of the case $\mu = -1$ being identical. When $\mu = +1$ in (1.5), we have

$$Q - P = H \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} - 1 \end{bmatrix}.$$

Consequently, by the fact that H is orthogonal, by $\tilde{x}^2 + \tilde{y}^2 + \tilde{z}^2 = 1$, and by (1.11),

$$|Q - P| = \sqrt{\tilde{x}^2 + \tilde{y}^2 + (\tilde{z} - 1)^2} = \sqrt{2 - 2\tilde{z}} = 2\sin\frac{\theta}{2}.$$

We also have, with $\mu = +1$ in (1.5),

$$\mathbf{n}_Q = Q = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = H \begin{bmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{bmatrix}.$$

Consequently, again by the fact that H is orthogonal, by $\tilde{x}^2 + \tilde{y}^2 + \tilde{z}^2 = 1$, and by (1.11),

$$(Q - P)\bullet\mathbf{n}_Q = \tilde{x}^2 + \tilde{y}^2 + (\tilde{z} - 1)\tilde{z} = 1 - \tilde{z} = 2\left(\sin\frac{\theta}{2}\right)^2.$$

Therefore,

$$\frac{1}{|Q - P|} = \frac{1}{2\sin(\theta/2)} \quad \text{and} \quad \frac{(Q - P)\bullet\mathbf{n}_Q}{|Q - P|^3} = \frac{1}{4\sin(\theta/2)}.$$

As a result, with $g(x, y, z) = g(Q)$ as in (1.3) and (1.4), and with $\mu = +1$ in (1.5), we have, respectively,

$$F(\theta, \phi) = g(x, y, z)\cos\frac{\theta}{2} \quad \text{(single-layer)},$$
$$F(\theta, \phi) = \frac{1}{2}\, g(x, y, z)\cos\frac{\theta}{2} \quad \text{(double-layer)}. \tag{2.1}$$

With $\mu = -1$ in (1.5), we have, similarly,

$$F(\theta, \phi) = g(x, y, z)\sin\frac{\theta}{2} \quad \text{(single-layer)},$$
$$F(\theta, \phi) = \frac{1}{2}\, g(x, y, z)\sin\frac{\theta}{2} \quad \text{(double-layer)}. \tag{2.2}$$

From this, we see that it is enough to treat the single-layer case when integrating over the surface of the unit sphere U; the double-layer integral is simply $1/2$ times the single-layer integral.

We now turn to $\widehat{T}_{n,n'}[f]$. Let us define

$$v(\theta) = \int_0^{2\pi} F(\theta, \phi)\, \mathrm{d}\phi, \quad \widehat{v}(t) = \int_0^{2\pi} \widehat{F}(t, \phi)\, \mathrm{d}\phi. \tag{2.3}$$

Thus,

$$\widehat{v}(t) = v(\Psi(t))\Psi'(t), \quad I[f] = \int_0^{\pi} v(\theta)\, \mathrm{d}\theta = \int_0^1 \widehat{v}(t)\, \mathrm{d}t. \tag{2.4}$$

By our assumption that $g(x, y, z)$ is infinitely differentiable over U, we have that it is infinitely differentiable also as a function of $\tilde{x}, \tilde{y}, \tilde{z}$. Thus, $F(\theta, \phi)$ is infinitely differentiable as a function of both θ and ϕ, and also 2π-periodic as a function of ϕ for $\phi \in (-\infty, \infty)$. Thus, the developments of [11, Section 3] apply, and we have that

$$\widehat{T}_{n,n'}[f] = \widetilde{T}_n[f] + \mathrm{O}(h'^{\nu}) \quad \text{as } h' \to 0 \quad \text{for every } \nu > 0. \tag{2.5}$$

where

$$\widetilde{T}_n[f] = h \sum_{j=0}^{n}{}'' \int_0^{2\pi} \widehat{F}(jh, \phi)\, \mathrm{d}\phi = h \sum_{j=0}^{n}{}'' \widehat{v}(jh). \tag{2.6}$$

(Recall that the double prime on the summation means that the first and the last terms are being halved.) Thus, if we let $n' \sim \alpha n^{\beta}$ as $n \to \infty$ for some fixed positive α and β, then (2.5) becomes

$$\widehat{T}_{n,n'}[f] = \widetilde{T}_n[f] + \mathrm{O}(h^{\nu}) \quad \text{as} \quad h \to 0 \quad \text{for every} \quad \nu > 0. \tag{2.7}$$

In the sequel, we let $n' \sim \alpha n^{\beta}$ as $n \to \infty$.

As is clear from (2.7), the error in $\widehat{T}_{n,n'}[f]$, as $h \to 0$, has the same asymptotic expansion as that of $\widetilde{T}_n[f]$. Thus, we need to concern ourselves only with the asymptotic expansion as $h \to 0$ of $\widetilde{T}_n[f]$, the trapezoidal rule approximation to the integral $\int_0^1 \widehat{v}(t)\, \mathrm{d}t$. For this, we need to study $\widehat{v}(t)$ as $t \to 0+$ and $t \to 1-$, in [11, Theorem A.2] (or, equivalently, [10, Theorem 4.1]). This we do by expanding $v(\theta)$ about $\theta = 0$ and π, for which we need to expand $F(\theta, \phi)$ about $\theta = 0$ and π. Following that, we employ the results of [10].

Throughout, we make use of the fact that the sequence $\{(\sin\theta)^i\}_{i=1}^{\infty}$ is a bona fide asymptotic scale both as $\theta \to 0$ and as $\theta \to \pi$.

3. Asymptotic expansions of $F(\theta, \phi)$ and $v(\theta)$

We now turn to the asymptotic expansion of $F(\theta, \phi)$ and $v(\theta)$ as $\theta \to 0$ and $\theta \to \pi$. For $\mu = +1$, $\theta = 0$ and π correspond to $(\tilde{x}, \tilde{y}, \tilde{z}) = (0, 0, 1)$ and $(\tilde{x}, \tilde{y}, \tilde{z}) = (0, 0, -1)$, respectively. Let us define $u(\tilde{x}, \tilde{y}, \tilde{z}) \equiv g(x, y, z)$. At the points $(0, 0, \pm 1)$, $u(\tilde{x}, \tilde{y}, \tilde{z})$ has the asymptotic expansions

$$u(\tilde{x}, \tilde{y}, \tilde{z}) \sim \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty} \frac{u^{(i,j,k)}(0,0,1)}{i!\,j!\,k!}\tilde{x}^i\tilde{y}^j(\tilde{z}-1)^k \quad \text{as } \theta \to 0,$$

$$u(\tilde{x}, \tilde{y}, \tilde{z}) \sim \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty} \frac{u^{(i,j,k)}(0,0,-1)}{i!\,j!\,k!}\tilde{x}^i\tilde{y}^j(\tilde{z}+1)^k \quad \text{as } \theta \to \pi,$$

where

$$u^{(i,j,k)}(\tilde{x}_0, \tilde{y}_0, \tilde{z}_0) = \left.\frac{\partial^{i+j+k}u}{\partial\tilde{x}^i\partial\tilde{x}^j\partial\tilde{z}^k}\right|_{(\tilde{x},\tilde{y},\tilde{z})=(\tilde{x}_0,\tilde{y}_0,\tilde{z}_0)}.$$

These are simply the Taylor series expansions of $u(\tilde{x}, \tilde{y}, \tilde{z})$ about $(0, 0, \pm 1)$. Using the short-hand notation $\sum_{i,j,k\geqslant 0} = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}$, and invoking (1.11), these expansions can be rewritten in the form

$$\begin{aligned} u(\tilde{x}, \tilde{y}, \tilde{z}) &\sim \sum_{i,j,k\geqslant 0} e_{i,j,k}^{(+)}(\cos\phi)^i(\sin\phi)^j(\sin\theta)^{i+j}(\cos\theta-1)^k \quad \text{as } \theta \to 0, \\ u(\tilde{x}, \tilde{y}, \tilde{z}) &\sim \sum_{i,j,k\geqslant 0} e_{i,j,k}^{(-)}(\cos\phi)^i(\sin\phi)^j(\sin\theta)^{i+j}(\cos\theta+1)^k \quad \text{as } \theta \to \pi, \end{aligned} \tag{3.1}$$

where

$$e_{i,j,k}^{(\pm)} = \frac{u^{(i,j,k)}(0,0,\pm 1)}{i!\,j!\,k!}. \tag{3.2}$$

As for the asymptotic expansions of $v(\theta)$, we can obtain these by substituting those of $F(\theta, \phi)$ in the integral $\int_0^{2\pi} F(\theta, \phi)\,d\phi$, and interchanging the order of integration and summation (which is allowed because the integration is over the finite interval $[0, \pi]$). By [11, Lemma 3.1], which, in our case, simply says that

$$\int_0^{2\pi}(\cos\phi)^i(\sin\phi)^j\,d\phi = 0 \quad \text{when } i \text{ or } j \text{ or both odd integers,}$$

we obtain the next two results, the first of which is for $\mu = +1$, while the second is for $\mu = -1$:

Theorem 3.1. *When $g(x, y, z)$ is infinitely smooth over U and $\mu = +1$ in* (1.5), *for the single-layer integral, $v(\theta) = \int_0^{2\pi} F(\theta, \phi)\, d\phi$ has the asymptotic expansions*

$$v(\theta) \sim \sum_{i,j,k \geqslant 0} A^{(+)}_{i,j,k} \cos(\theta/2)(\sin\theta)^{2i+2j}(\cos\theta - 1)^k \quad as\ \theta \to 0,$$
$$v(\theta) \sim \sum_{i,j,k \geqslant 0} A^{(-)}_{i,j,k} \cos(\theta/2)(\sin\theta)^{2i+2j}(\cos\theta + 1)^k \quad as\ \theta \to \pi, \tag{3.3}$$

where $A^{(\pm)}_{i,j,k}$ are constants given by

$$A^{(\pm)}_{i,j,k} = e^{(\pm)}_{2i,2j,k} \int_0^{2\pi} (\cos\phi)^{2i}(\sin\phi)^{2j}\, \mathrm{d}\phi, \quad i, j, k = 0, 1, \ldots\ .$$

Consequently,

$$v(\theta) \sim \sum_{i=0}^{\infty} c^{(+)}_i \theta^{2i} \quad as\ \theta \to 0; \quad v(\theta) \sim \sum_{i=0}^{\infty} c^{(-)}_i (\pi - \theta)^{2i+1} \quad as\ \theta \to \pi \tag{3.4}$$

for some constants $c^{(\pm)}_i$.

Theorem 3.2. *When $g(x, y, z)$ is infinitely smooth over U and $\mu = -1$ in* (1.5), *for the single-layer integral, $v(\theta) = \int_0^{2\pi} F(\theta, \phi)\, \mathrm{d}\phi$* has the asymptotic expansions

$$v(\theta) \sim \sum_{i,j,k \geqslant 0} A^{(+)}_{i,j,k} \sin(\theta/2)(\sin\theta)^{2i+2j}(\cos\theta - 1)^k \quad as\ \theta \to 0,$$
$$v(\theta) \sim \sum_{i,j,k \geqslant 0} A^{(-)}_{i,j,k} \sin(\theta/2)(\sin\theta)^{2i+2j}(\cos\theta + 1)^k \quad as\ \theta \to \pi, \tag{3.5}$$

where $A^{(\pm)}_{i,j,k}$ are constants given by

$$A^{(\pm)}_{i,j,k} = e^{(\pm)}_{2i,2j,k} \int_0^{2\pi} (\cos\phi)^{2i}(\sin\phi)^{2j}\, \mathrm{d}\phi, \quad i, j, k = 0, 1, \ldots\ .$$

Consequently,

$$v(\theta) \sim \sum_{i=0}^{\infty} c^{(+)}_i \theta^{2i+1} \quad as\ \theta \to 0; \quad v(\theta) \sim \sum_{i=0}^{\infty} c^{(-)}_i (\pi - \theta)^{2i} \quad as\ \theta \to \pi \tag{3.6}$$

for some constants $c^{(\pm)}_i$.

Remark. Note that $c^{(\pm)}_0$ in both theorems are proportional to $e^{(\pm)}_{0,0,0}$. Therefore, if any one of the $e^{(\pm)}_{0,0,0} = u(0, 0, \pm 1) = g(\pm\mu P)$ vanishes, then the corresponding $c^{(\pm)}_0$ vanishes as well. We make use of this observation in Section 5 to design numerical integration rules with very high accuracy.

4. Asymptotic expansion of $\widehat{T}_{n,n'}[f]$

We now analyze the asymptotic behavior of $\widehat{T}_{n,n'}[f]$ for the two choices of $\Psi(t)$ described in Section 1. Below, $\psi(t)$ is a function in the extended class $\mathscr{S}_m$.

We would like to emphasize that the better of the results given in Theorems 4.1 and 4.2 and also in Theorem 5.1 are made possible by the fact that the powers of t and $(1-t)$ in the asymptotic expansions of $\psi'(t)$ given in (1.15) increase by 2 instead of by 1.

Theorem 4.1. *Let $\psi(t)$ be in $\mathscr{S}_m$. With $\Psi(t)=\Psi_1(t)=\pi\psi(t)$ and with $n'\sim\alpha n^\beta$ as $n\to\infty$ for some fixed positive α and β, there holds*

$$\widehat{T}_{n,n'}[f]-I[f]=\begin{cases}\mathrm{O}(h^{2m+2}) & \text{as } h\to 0 \quad \text{if } m \text{ even integer},\\ \mathrm{O}(h^{m+1}) & \text{as } h\to 0 \quad \text{otherwise}.\end{cases}$$

For m an even integer, we also have the complete Euler–Maclaurin expansion

$$\widehat{T}_{n,n'}[f]\sim I[f]+\sum_{i=0}^{\infty}\sigma_i\,h^{2m+2+2i} \quad \text{as } h\to 0.$$

The proof of this theorem can be achieved by invoking [10, Theorem 4.1 and part (i) of Corollary 4.2] in conjunction with the asymptotic expansions of $v(\theta)$ as $\theta\to 0$ and $\theta\to\pi$. We leave the details of the proof to the reader. Note the better accuracy that $\widehat{T}_{n,n'}[f]$ can achieve when m is an even integer.

Note that, with $F(\theta,\phi)$ as in (2.1) and (2.2), and with $\widehat{F}(t,\phi)$ as in (1.13), in Theorem 4.1, $\widehat{F}(0,\phi)=\widehat{F}(1,\phi)=0$ when $m>0$; in such a case, $\widehat{T}_{n,n'}[f]$ becomes

$$\widehat{T}_{n,n'}[f]=hh'\sum_{j=1}^{n-1}\sum_{k=1}^{n'}\widehat{F}(jh,kh').$$

The next theorem shows that better convergence rates can be obtained from $\widehat{T}_{n,n'}[f]$ if we use the transformation $\Psi_2(t)$ as described in Section 1.

Theorem 4.2. *Let $\psi(t)$ be in $\mathscr{S}_m$.* With *$\Psi(t)=\Psi_2(t)=2\pi\psi(t/2)$ when $\mu=-1$ in* (1.5), *or $\Psi(t)=\Psi_2(t)=\pi[2\psi((1+t)/2)-1]$ when $\mu=+1$ in* (1.5), *and with $n'\sim\alpha n^\beta$ as $n\to\infty$ for some fixed positive α* and *β, there holds*

$$\widehat{T}_{n,n'}[f]-I[f]=\begin{cases}\mathrm{O}(h^{4m+4}) & \text{as } h\to 0 \quad \text{if } 2m \text{ odd integer},\\ \mathrm{O}(h^{2m+2}) & \text{as } h\to 0 \quad \text{otherwise}.\end{cases}$$

For $2m$ an odd integer, we also have the complete Euler–Maclaurin expansion

$$\widehat{T}_{n,n'}[f]\sim I[f]+\sum_{i=0}^{\infty}\sigma_i\,h^{4m+4+2i} \quad \text{as } h\to 0.$$

The proof of this theorem can be achieved by invoking [10, Theorem 4.4] in conjunction with the asymptotic expansions of $v(\theta)$ as $\theta\to 0$ and $\theta\to\pi$. We leave the details of the proof to the reader. The

Table 1
Relative errors in the rules $\widehat{T}_n[f] = \widehat{T}_{n,n}[f]$ for the integral of Section 4.1, obtained with $n = 2^k$, $k = 1(1)9$, and with the transformation $\Psi(t) = \Psi_1(t)$, using $m = 1(1)8$

n	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$	$m=6$	$m=7$	$m=8$
2	$2.40D+01$	$1.94D+01$	$1.55D+01$	$1.22D+01$	$9.19D+00$	$6.44D+00$	$3.90D+00$	$1.52D+00$
4	$2.74D+00$	$8.34D+00$	$1.14D+01$	$1.21D+01$	$1.15D+01$	$1.02D+01$	$8.50D+00$	$6.73D+00$
8	$1.47D-02$	$6.96D-03$	$2.66D-01$	$9.56D-01$	$1.97D+00$	$3.17D+00$	$4.43D+00$	$5.66D+00$
16	$6.11D-04$	$2.05D-05$	$6.19D-05$	$7.64D-04$	$3.28D-03$	$7.56D-03$	$1.11D-02$	$9.34D-03$
32	$3.34D-04$	$3.01D-07$	$5.75D-07$	$6.00D-11$	$3.80D-09$	$9.02D-09$	$5.91D-08$	$1.85D-07$
64	$9.49D-05$	$4.68D-09$	$3.57D-08$	$5.56D-14$	$5.13D-11$	$3.71D-18$	$1.52D-13$	$5.95D-20$
128	$2.44D-05$	$7.30D-11$	$2.23D-09$	$5.40D-17$	$8.00D-13$	$2.23D-22$	$5.91D-16$	$3.03D-27$
256	$6.15D-06$	$1.14D-12$	$1.39D-10$	$5.27D-20$	$1.25D-14$	$1.35D-26$	$2.30D-18$	$1.85D-32$
512	$1.54D-06$	$1.78D-14$	$8.71D-12$	$5.14D-23$	$1.95D-16$	$8.50D-31$	$9.00D-21$	$0.00D+00$

Table 2
The numbers $\mu_{m,k} = 1/\log 2 \cdot \log(|\widehat{T}_{2^k}[f] - I[f]|/|\widehat{T}_{2^{k+1}}[f] - I[f]|)$ for $k = 1(1)8$ and $m = 1(1)8$, for the integral of Section 4.1, where $\widehat{T}_n[f]$ are those of Table 1

k	$m=1$	$m=2$	$m=3$	$m=4$	$m=5$	$m=6$	$m=7$	$m=8$
1	3.129	1.216	0.444	0.005	−0.324	−0.656	−1.124	−2.148
2	7.547	10.226	5.422	3.666	2.543	1.678	0.939	0.251
3	4.584	8.407	12.070	10.289	9.234	8.714	8.639	9.242
4	0.870	6.092	6.751	23.604	19.716	19.677	17.522	15.624
5	1.817	6.006	4.010	10.074	6.214	31.178	18.570	41.498
6	1.958	6.001	4.001	10.008	6.002	14.025	8.006	24.228
7	1.990	6.000	4.000	10.002	6.001	14.006	8.001	17.322
8	1.997	6.000	4.000	10.001	6.000	13.958	8.000	*

asymptotic expansion of $v(\theta)$ at $\theta = 0$ when $\mu = +1$ or at $\theta = \pi$ when $\mu = -1$, that is, at the pole of the rotated U that is mapped to the point of singularity P, do not contribute anything to the asymptotic expansions of $\widehat{T}_{n,n'}[f]$.

Note the remarkable accuracy that $\widehat{T}_{n,n'}[f]$ can achieve when $2m$ is an odd integer. Obviously, the variable transformation in Theorem 4.2 is more effective than that of Theorem 4.1 for integration over U. In the next section, we show how to improve on the $\widehat{T}_{n,n'}[f]$ of Theorem 4.2.

4.1. A numerical example

We have applied the methods of this section to the integral in (1.2), $f(Q)$ having a single-layer singularity as in (1.3), and $g(x, y, z) = e^{x+2y+3z}$ and $P = (0, 0, -1)$. We have $I[f] = 40.90220018862976\cdots$. Also, we take $H = I$ in (1.5), so that $\mu = -1$ there. Of course, Theorems 4.1 and 4.2 apply to this case.

The numerical results in Tables 1–4, which were computed in quadruple-precision arithmetic, illustrate the result of both theorems very clearly. Tables 1 and 3 give the relative errors in the $\widehat{T}_n[f] \equiv \widehat{T}_{n,n}[f]$,

Table 3
Relative errors in the rules $\widehat{T}_n[f] = \widehat{T}_{n,n}[f]$ for the integral of Section 4.1, obtained with $n = 2^k$, $k = 1(1)9$, and with the transformation $\Psi(t) = \Psi_2(t)$, using $m = 1(0.5)4.5$.

n	$m=1$	$m=1.5$	$m=2$	$m=2.5$	$m=3$	$m=3.5$	$m=4$	$m=4.5$
2	$1.39D-02$	$7.23D-02$	$1.31D-02$	$1.74D-01$	$3.46D-01$	$4.99D-01$	$6.22D-01$	$7.18D-01$
4	$4.94D-03$	$2.16D-02$	$5.85D-02$	$7.09D-02$	$4.91D-02$	$6.12D-04$	$6.63D-02$	$1.36D-01$
8	$7.90D-05$	$1.40D-06$	$4.03D-06$	$2.32D-04$	$4.35D-04$	$2.33D-05$	$1.25D-03$	$3.01D-03$
16	$5.90D-06$	$3.00D-12$	$2.94D-08$	$8.27D-11$	$5.33D-11$	$5.38D-09$	$1.28D-08$	$3.99D-08$
32	$3.68D-07$	$2.97D-15$	$4.57D-10$	$1.53D-19$	$1.21D-12$	$4.04D-22$	$5.44D-15$	$7.20D-19$
64	$2.30D-08$	$2.89D-18$	$7.14D-12$	$9.22D-24$	$4.70D-15$	$1.02D-28$	$5.28D-18$	$3.27D-33$
128	$1.44D-09$	$2.82D-21$	$1.12D-13$	$5.61D-28$	$1.84D-17$	$5.78D-34$	$5.15D-21$	$3.85D-34$
256	$8.99D-11$	$2.76D-24$	$1.74D-15$	$3.39D-32$	$7.17D-20$	$9.63D-35$	$5.03D-24$	$0.00D+00$
512	$5.62D-12$	$2.69D-27$	$2.72D-17$	$5.78D-34$	$2.80D-22$	$0.00D+00$	$4.91D-27$	$0.00D+00$

Table 4
The numbers $\mu_{m,k} = \frac{1}{\log 2} \cdot \log(|\widehat{T}_{2^k}[f] - I[f]|/|\widehat{T}_{2^{k+1}}[f] - I[f]|)$ for $k = 1(1)9$ and $m = 1(0.5)4.5$, for the integral of Section 4.1, where $\widehat{T}_n[f]$ are those of Table 3

k	$m=1$	$m=1.5$	$m=2$	$m=2.5$	$m=3$	$m=3.5$	$m=4$	$m=4.5$
1	1.492	1.744	−2.160	1.296	2.818	9.671	3.231	2.397
2	5.968	13.912	13.826	8.254	6.818	4.715	5.734	5.500
3	3.742	18.832	7.099	21.421	22.960	12.080	16.571	16.206
4	4.001	9.980	6.006	29.012	5.465	43.599	21.165	35.689
5	4.000	10.005	6.001	14.017	8.004	21.917	10.008	47.644
6	4.000	10.001	6.000	14.004	8.001	17.429	10.002	3.087
7	4.000	10.000	6.000	14.014	8.000	2.585	10.001	3.087
8	4.000	10.000	6.000	5.874	8.000	2.585	10.000	3.087

$n = 2^k$, $k = 1, 2, \ldots, 9$, for various values of m. Tables 2 and 4 present the numbers

$$\mu_{m,k} = \frac{1}{\log 2} \cdot \log \left(\frac{|\widehat{T}_{2^k}[f] - I[f]|}{|\widehat{T}_{2^{k+1}}[f] - I[f]|} \right)$$

for the same values of m and for $k = 1, 2, \ldots, 8$. It is seen that from Table 2 that, when the basic method with $\Psi(t) = \Psi_1(t)$ is used, then the $\mu_{m,k}$ are tending to $2m + 2$ when m is an even integer and to $m + 1$ otherwise, completely in accordance with Theorem 4.1. Similarly, we see from Table 4 that, when the basic method with $\Psi(t) = \Psi_2(t)$ is used, then the $\mu_{m,k}$ are tending to $4m + 4$ when $2m$ is an odd integer and to $2m + 2$ otherwise, completely in accordance with Theorem 4.2.

In connection with the computation of $\Psi_1(t) = \pi\psi(t)$ and $\Psi_2(t) = 2\pi\psi(t/2)$ or $\Psi_2(t) = \pi[2\psi((1 + t)/2) - 1]$, with $0 \leqslant t \leqslant 1$, we would like to note the following: For $\Psi_1(t)$, we need to do the actual computation of $\psi(t)$ for $0 \leqslant t \leqslant 1/2$ and make use of (1.20) for $1/2 \leqslant t \leqslant 1$. Similarly, for $\Psi_2(t)$, we need to compute $\psi(t)$ only for $0 \leqslant t \leqslant 1/2$. Consequently, there is no extra complication or cost in the computation of $\Psi_2(t)$ relative to that of $\Psi_1(t)$.

5. Further improvement for $\widehat{T}_{n,n'}[f]$

In Theorem 4.2 of the preceding section, we showed that, with $\Psi(t) = \Psi_2(t)$, $\widehat{T}_{n,n'}[f]$ produces very accurate approximations to $I[f]$ when $2m$ is an odd integer. In this section, we continue our treatment of this case by improving further the performance of the rule $\widehat{T}_{n,n'}$. As mentioned following [10, Definition 1.1; 11, Appendix C], it is desirable to get as much accuracy out of $\widehat{T}_{n,n'}[f]$ for a given value of m hence for a given amount of clustering of the transformed abscissas on U. As in the preceding section, this can be achieved for special values of m, provided the integrand is preprocessed suitably. This preprocessing is performed by recalling the remark at the end of Section 3.

Let us subtract $u(0, 0, -\mu)$ from the function $u(\tilde{x}, \tilde{y}, \tilde{z})$; by (1.5), this amounts to subtracting $g(-P)$ from $g(Q)$. Then,

$$I[f] = I_1 + I_2; \quad I_1 = \int\int_U [g(Q) - g(-P)]V(Q)\,\mathrm{d}A, \quad I_2 = g(-P)\int\int_U V(Q)\,\mathrm{d}A,$$

where $V(Q)$ stands for the singular factor of $f(Q)$, that is, $V(Q) = f(Q)/g(Q)$,

$$V(Q) = \frac{1}{|Q-P|} \quad \text{(single-layer)}, \qquad V(Q) = \frac{(Q-P)\cdot \mathbf{n}_Q}{|Q-P|^3} \quad \text{(double-layer)}.$$

Also, by the developments of Section 2,

$$E = \int\int_U V(Q)\,\mathrm{d}A = 4\pi \quad \text{(single-layer)}, \qquad E = \int\int_U V(Q)\,\mathrm{d}A = 2\pi \quad \text{(double-layer)}.$$

We next apply the rule $\widehat{T}_{n,n'}$ to the function $f^{\mathrm{imp}}(Q) = [g(Q) - g(-P)]V(Q)$ with $\Psi(t) = \Psi_2(t)$. The resulting approximation $\check{T}_{n,n'}[f]$ for $I[f]$ then is

$$\check{T}_{n,n'}[f] = \widehat{T}_{n,n'}[f^{\mathrm{imp}}] + Eg(-P). \tag{5.1}$$

If we let $F^{\mathrm{imp}}(\theta, \phi) = f^{\mathrm{imp}}(Q)\sin\theta$, and $v^{\mathrm{imp}}(\theta) = \int_0^\pi F^{\mathrm{imp}}(\theta, \phi)\,\mathrm{d}\phi$, then $v^{\mathrm{imp}}(\theta)$, by Theorems 3.1 and 3.2, and by the remark at the end of Section 3, has the asymptotic expansions

$$\left.\begin{aligned} v^{\mathrm{imp}}(\theta) &\sim \sum_{i=0}^{\infty} c_i^{(+)}\theta^{2i} \quad \text{as } \theta \to 0 \\ v^{\mathrm{imp}}(\theta) &\sim \sum_{i=1}^{\infty} c_i^{(-)}(\pi-\theta)^{2i+1} \quad \text{as } \theta \to \pi \end{aligned}\right\} \quad (\mu = +1)$$

and

$$\left.\begin{aligned} v^{\mathrm{imp}}(\theta) &\sim \sum_{i=1}^{\infty} c_i^{(+)}\theta^{2i+1} \quad \text{as } \theta \to 0 \\ v^{\mathrm{imp}}(\theta) &\sim \sum_{i=0}^{\infty} c_i^{(-)}(\pi-\theta)^{2i} \quad \text{as } \theta \to \pi \end{aligned}\right\} \quad (\mu = -1).$$

Of course, the $c_i^{(\pm)}$ here are not necessarily those in (3.3) and (3.4). The important point to note is that the expansions of $v^{\mathrm{imp}}(\theta)$ containing the odd powers of θ and $\pi - \theta$ begin with the powers θ^3 and $(\pi-\theta)^3$, followed by the powers θ^5 and $(\pi-\theta)^5$, respectively. The ones containing the even powers remain of the same form as those of $v(\theta)$ in (3.3) and (3.4). Using these facts, we can obtain better approximations

Table 5
Relative errors in the rules $\check{T}_n[f] = \check{T}_{n,n}[f]$ for the integral of Section 4.1, obtained with $n = 2^k$, $k = 1(1)9$, and with the transformation $\Psi(t) = \Psi_2(t)$, using $m = 0.25(0.25)2.25$

n	$m = 0.25$	$m = 0.5$	$m = 0.75$	$m = 1$	$m = 1.25$	$m = 1.5$	$m = 1.75$	$m = 2$	$m = 2.25$
2	4.42D − 01	3.28D − 01	1.73D − 01	3.98D − 02	4.04D − 02	6.06D − 02	2.59D − 02	5.33D − 02	1.66D − 01
4	1.08D − 02	9.05D − 03	8.80D − 05	3.41D − 03	4.71D − 03	2.16D − 02	4.13D − 02	5.84D − 02	6.89D − 02
8	1.46D − 05	1.26D − 05	1.35D − 05	1.58D − 05	1.45D − 05	1.40D − 06	1.84D − 05	2.12D − 06	8.95D − 05
16	4.03D − 09	1.92D − 08	6.15D − 12	1.71D − 10	5.45D − 14	2.56D − 12	7.65D − 14	5.80D − 12	7.22D − 12
32	2.16D − 11	3.00D − 10	4.24D − 15	6.61D − 13	2.21D − 18	2.55D − 15	2.42D − 21	1.52D − 17	4.87D − 24
64	1.19D − 13	4.69D − 12	2.92D − 18	2.58D − 15	1.89D − 22	2.48D − 18	2.57D − 26	3.69D − 21	6.38D − 30
128	6.56D − 16	7.32D − 14	2.02D − 21	1.01D − 17	1.63D − 26	2.42D − 21	2.83D − 31	9.00D − 25	2.89D − 33
256	3.62D − 18	1.14D − 15	1.39D − 24	3.93D − 20	1.40D − 30	2.36D − 24	6.84D − 33	2.20D − 28	1.73D − 33
512	2.00D − 20	1.79D − 17	9.62D − 28	1.54D − 22	1.04D − 32	2.31D − 27	6.16D − 33	6.11D − 32	2.89D − 33

than those discussed in Theorem 4.2 by employing the transformation $\Psi_2(t)$. This is the subject of the next theorem.

Theorem 5.1. *Let $\psi(t)$ be in $\mathscr{S}_m$. With $\Psi(t) = \Psi_2(t) = 2\pi\psi(t/2)$ when $\mu = -1$ in* (1.5), *or $\Psi(t) = \Psi_2(t) = \pi[2\psi((1+t)/2) - 1]$ when $\mu = +1$ in* (1.5), *and with $n' \sim \alpha n^\beta$ as $n \to \infty$ for some fixed positive α and β, there holds*

$$\check{T}_{n,n'}[f] - I[f] = \begin{cases} O(h^{6m+6}) & \text{as } h \to 0 \quad if\ 4m\ odd\ integer, \\ O(h^{4m+4}) & \text{as } h \to 0 \quad otherwise. \end{cases}$$

For $4m$ an odd integer, we also have the complete Euler–Maclaurin expansion

$$\check{T}_{n,n'}[f] \sim I[f] + \sum_{i=0}^{\infty} \sigma_i h^{6m+6+2i} + \sum_{i=0}^{\infty} \sigma_i' h^{8m+8+2i} + \sum_{i=0}^{\infty} \sigma_i'' h^{10m+10+2i} \quad \text{as } h \to 0.$$

For example, in case $m = 0.25$, the expansion in this theorem contains the powers $h^{7.5}, h^{9.5}, h^{10}, h^{11.5}, h^{12}, h^{12.5}, \ldots$.

Finally, one of $F^{\text{imp}}(0,\phi)$ and $F^{\text{imp}}(\pi,\phi)$ is zero and the other one is independent of ϕ. [Actually, $F^{\text{imp}}(\pi,\phi) \equiv 0$ when $\mu = +1$, and $F^{\text{imp}}(0,\phi) \equiv 0$ when $\mu = -1$.] This observation can be used to conclude that the number of integrand evaluations in $\check{T}_{n,n'}[f]$ as given by (5.1) [and by (1.14)] can be reduced by $2n'$.

5.1. A numerical example

We have applied the improved method above to the example of Section 4.1. Of course, Theorem 5.1 applies to this case.

The numerical results in Tables 5 and 6, which were computed in quadruple-precision arithmetic, illustrate the result of this theorem very clearly. Table 5 gives the relative errors in the $\check{T}_n[f] \equiv \check{T}_{n,n}[f]$,

Table 6
The numbers $\mu_{m,k} = 1/\log 2 \cdot \log(|\check{T}_{2^k}[f] - I[f]|/|\check{T}_{2^{k+1}}[f] - I[f]|)$ for $k = 1(1)9$ and $m = 0.25(0.25)2.25$, for the integral of Section 4.1, where $\check{T}_n[f]$ are those of Table 5

k	$m = 0.25$	$m = 0.5$	$m = 0.75$	$m = 1$	$m = 1.25$	$m = 1.5$	$m = 1.75$	$m = 2$	$m = 2.25$
1	5.361	5.179	10.937	3.544	3.101	1.488	−0.674	−0.131	1.270
2	9.522	9.494	2.701	7.756	8.341	13.913	11.130	14.751	9.588
3	11.827	9.351	21.070	16.496	27.989	19.061	27.844	18.477	23.563
4	7.541	6.002	10.503	8.012	14.591	9.974	24.914	18.539	40.432
5	7.507	6.001	10.502	8.002	13.509	10.005	16.522	12.010	19.542
6	7.501	6.000	10.501	8.001	13.502	10.001	16.470	12.002	11.108
7	7.500	6.000	10.500	8.000	13.511	10.000	5.373	12.001	0.737
8	7.500	6.000	10.500	8.000	7.069	10.000	0.150	11.813	−0.737

$n = 2^k,\ k = 1, 2, \ldots, 9,$ for various values of m. Table 6 presents the numbers

$$\mu_{m,k} = \frac{1}{\log 2} \cdot \log\left(\frac{|\check{T}_{2^k}[f] - I[f]|}{|\check{T}_{2^{k+1}}[f] - I[f]|}\right)$$

for the same values of m and for $k = 1, 2, \ldots, 8$. It is seen that, with increasing k, the $\mu_{m,k}$ are tending to $6m + 6$ when $4m$ an odd integer, that is, when $m = j/2 - 3/4,\ j = 1, 2, \ldots,$ and to $4m + 4$ otherwise, completely in accordance with Theorem 5.1.

6. Numerical integration of regular integrands over U

In the paper [11], we treated the numerical integration of regular functions over smooth surfaces that are homeomorphic to the surface of the unit sphere. Of course, this treatment includes numerical integration over U as a special case. For the sake of completeness, in this section, we summarize the developments of [11] for this special case.

We would like to compute numerically $I[f] = \int\int_U f(Q)\,\mathrm{d}A$, when $f(Q) = f(x, y, z)$ is a regular integrand. Switching to the spherical coordinates θ and ϕ,

$$(x, y, z) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta),$$

we write this integral in the form

$$I[f] = \int_0^{\pi}\left[\int_0^{2\pi} F(\theta, \phi)\,\mathrm{d}\phi\right]\mathrm{d}\theta; \qquad F(\theta, \phi) = f(x, y, z)\sin\theta.$$

Using the variable transformation $\theta = \Psi(t) = \Psi_1(t) = \pi\psi(t)$, where $\psi \in \mathscr{S}_m$, we re-express $I[f]$ as in

$$I[f] = \int_0^{1}\left[\int_0^{2\pi} \widehat{F}(t, \phi)\,\mathrm{d}\phi\right]\mathrm{d}t; \qquad \widehat{F}(t, \phi) = F(\Psi(t), \phi)\Psi'(t).$$

We then approximate $I[f]$ via the rule

$$\widehat{T}_{n,n'}[f] = hh' \sum_{j=1}^{n-1} \sum_{k=1}^{n'} \widehat{F}(jh, kh'); \quad h = \frac{1}{n}, \quad h' = \frac{2\pi}{n'}.$$

The error in this approximation satisfies

$$\widehat{T}_{n,n'}[f] - I[f] = \begin{cases} O(h^{4m+4}) & \text{as } h \to 0 \quad \text{if } 2m \text{ odd integer}, \\ O(h^{2m+2}) & \text{as } h \to 0 \quad \text{otherwise}. \end{cases}$$

This rule can be improved as follows: Let $B = [f(0, 0, 1) + f(0, 0, -1)]/2$. The improved rule $\check{T}_{n,n'}[f]$ is given as in

$$\check{T}_{n,n'}[f] = \widehat{T}_{n,n'}[f] + 4\pi B - 2\pi B \left[h \sum_{j=1}^{n-1} \sin(\Psi(j/n))\Psi'(j/n) \right].$$

The error in this approximation satisfies

$$\check{T}_{n,n'}[f] - I[f] = \begin{cases} O(h^{6m+6}) & \text{as } h \to 0 \quad \text{if } 4m \text{ odd integer}, \\ O(h^{4m+4}) & \text{as } h \to 0 \quad \text{otherwise}. \end{cases}$$

For $4m$ an odd integer, we also have the complete Euler–Maclaurin expansion

$$\check{T}_{n,n'}[f] \sim I[f] + \sum_{i=0}^{\infty} \sigma_i \, h^{6m+6+2i} + \sum_{i=0}^{\infty} \sigma'_i h^{8m+8+2i} + \sum_{i=0}^{\infty} \sigma''_i \, h^{10m+10+2i} \quad \text{as } h \to 0.$$

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